

## (2E)-1-(2,5-Dimethylthiophen-3-yl)-3-(3-nitrophenyl)prop-2-en-1-one

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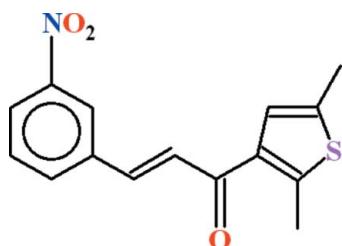
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Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(C-C) = 0.004$  Å;  $R$  factor = 0.047;  $wR$  factor = 0.117; data-to-parameter ratio = 13.5.

In the title compound,  $C_{15}H_{13}NO_3S$ , the benzene ring and the five-membered heterocyclic ring are oriented at a dihedral angle of  $12.00(6)^\circ$ . In the crystal,  $C-H\cdots O$  interactions generate two types of cyclic motifs,  $R_2^2(14)$  and  $R_2^2(26)$ , connecting the molecules into tapes extending along [101]. In addition, there are  $\pi-\pi$  stacking interactions between the benzene and thiophene rings with centroid-centroid distances of  $3.7263(14)$  and  $3.7487(14)$  Å.

## Related literature

For the synthesis of similar compounds, see: Asiri & Khan (2010, 2011); Kalirajan *et al.* (2009); Patil *et al.* (2009); Sarojini *et al.* (2006). For related structures and background references, see: Asiri *et al.* (2010a,b). For graph-set notation, see: Bernstein *et al.* (1995).



## Experimental

## Crystal data

$C_{15}H_{13}NO_3S$   
 $M_r = 287.32$   
Monoclinic,  $P2_1/c$

$a = 7.3802(5)$  Å  
 $b = 13.7973(9)$  Å  
 $c = 13.4638(8)$  Å

$\beta = 96.997(3)^\circ$   
 $V = 1360.77(15)$  Å<sup>3</sup>  
 $Z = 4$   
Mo  $K\alpha$  radiation

$\mu = 0.24$  mm<sup>-1</sup>  
 $T = 296$  K  
 $0.25 \times 0.22 \times 0.20$  mm

## Data collection

Bruker KAPPA APEXII CCD diffractometer  
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)  
 $T_{\min} = 0.945$ ,  $T_{\max} = 0.955$

10732 measured reflections  
2466 independent reflections  
1493 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.051$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.047$   
 $wR(F^2) = 0.117$   
 $S = 1.03$   
2466 reflections

183 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.17$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.25$  e Å<sup>-3</sup>

**Table 1**  
Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$               | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-----------------------------|-------|-------------|-------------|---------------|
| C6—H6···O3 <sup>i</sup>     | 0.93  | 2.46        | 3.373 (3)   | 168           |
| C15—H15B···O2 <sup>ii</sup> | 0.96  | 2.59        | 3.339 (4)   | 135           |

Symmetry codes: (i)  $-x, -y, -z$ ; (ii)  $-x + 1, -y, -z + 1$ .

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2432).

## References

Asiri, A. M. & Khan, S. A. (2010). *Molbank*, M687.  
Asiri, A. M. & Khan, S. A. (2011). *Molecules*, **16**, 523–531.  
Asiri, A. M., Khan, S. A. & Tahir, M. N. (2010a). *Acta Cryst. E66*, o2358.  
Asiri, A. M., Khan, S. A. & Tahir, M. N. (2010b). *Acta Cryst. E66*, o2404.  
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.  
Bruker (2005). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.  
Bruker (2009). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.  
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.  
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.  
Kalirajan, R., Sivakumar, S. U., Jubie, S., Gowramma, B. & Suresh, B. (2009). *Int. J. ChemTech Res.* **1**, 27–34.  
Patil, C. B., Mahajan, S. K. & Katti, S. A. (2009). *J. Pharm. Sci. Res.* **1**, 11–22.  
Sarojini, B. K., Narayana, B., Ashalatha, B. V., Indira, J. K. G. & Lobo, K. G. (2006). *J. Cryst. Growth*, **295**, 54–59.  
Sheldrick, G. M. (2008). *Acta Cryst. A64*, 112–122.  
Spek, A. L. (2009). *Acta Cryst. D65*, 148–155.